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14. ABSTRACT The workshop on "Roaming and Cold Molecules" was held at Emory university Oct. 8-9, 2016. There were 17 invited talks and more than 60 participants took part. The unusual "roaming" pathway was discussed in roughly half the talks. Collision dynamics at very low energies was the focus of four talks and the remaining talks focused on advances in electronic structure theory and unusual reaction dynamics related to roaming. The speakers were all at the top of these fields and the graduate students and postdocs who attended were thus exposed to state-of-the-art research.					
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a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU			19b. TELEPHONE NUMBER 404-727-6592

## Report Title

Final Report: Workshop on Roaming and Cold Molecule Dynamics

### ABSTRACT

The workshop on "Roaming and Cold Molecules" was held at Emory university Oct. 8-9, 2016. There were 17 invited talks and more than 60 participants took part.

The unusual "roaming" pathway was discussed in roughly half the talks. Collision dynamics at very low energies was the focus of four talks and the remaining talks focused on advances in electronic structure theory and unusual reaction dynamics related to roaming. The speakers were all at the top of these fields and the graduate students and postdocs who attended were thus exposed to state-of-the art research.

New connections were made at this workshop and these will likely result in fruitful new collaborations.

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**(a) Papers published in peer-reviewed journals (N/A for none)**

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Paper

**TOTAL:**

**Number of Papers published in peer-reviewed journals:**

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Received

Paper

**TOTAL:**

**Number of Papers published in non peer-reviewed journals:**

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**(c) Presentations**

Number of Presentations:

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**Non Peer-Reviewed Conference Proceeding publications (other than abstracts):**

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Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

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**Peer-Reviewed Conference Proceeding publications (other than abstracts):**

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Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

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**(d) Manuscripts**

Received      Paper

**TOTAL:**

Number of Manuscripts:

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**Books**

Received      Book

**TOTAL:**

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

### Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: .....

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:.....

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:.....

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):.....

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### Names of Personnel receiving masters degrees

NAME

**Total Number:**

### Names of personnel receiving PHDs

NAME

**Total Number:**

### Names of other research staff

NAME

PERCENT SUPPORTED

**FTE Equivalent:**

**Total Number:**

### Sub Contractors (DD882)

### Inventions (DD882)

### Scientific Progress

The workshop achieved the desired goal of bringing many of the world's experts studying roaming to Emory. Several outstanding speakers also represented the area of cold molecules. Student an postdocs present were exposed to the state of the art in these two "hot" areas of research.

### Technology Transfer

## **Final Report Narrative for Roaming Workshop**

This workshop took place Oct 8-9, 2016 at Emory University. The program and list of attendees (nearly 60) from around the world are given below.

The workshop followed immediately one on Ultracold Molecules, also held at Emory. Several people spoke at both workshops as there is significant interest in roaming in the cold molecule community.

The interest in roaming, which remains high, stems from the unusual roaming pathway in which an energized molecule appears to be decomposing into radical products, but instead undergoes an atom abstraction at long range to make molecular products. The workshop covered numerous aspects of this pathway, from complete classical trajectory simulations to analytical non-linear dynamics theories of roaming to attempts to extend conventional transition state theory to describe roaming. Experimentally, there are only indirect diagnostics of roaming. Often experiments require corresponding high-level simulations to confirm the presence of roaming in the experiment. There was some discussion about how roaming might be directly observed in experiment. It appears that time dependent measurements might be one route, as roaming does occur on a slower time scale than the direct pathway to molecular products.

Several new collaborations may have resulted from the workshop. I currently have a postdoctoral associate visiting my group investigating simple models of roaming reactions. This appears to be a new direction in the field and this was "kicked off" in a talk by Prof. Wiggins, who presented an interesting model developed by his collaborator, Prof. Carpenter.

ARO Workshop on Roaming and Cold Molecules  
Emory University, 360 Atwood Hall

Schedule for **SATURDAY**, Oct. 8, 2016

AM Session Chairs: Craig Murray and Phillip Stancil

8:30 – 9:00	Continental Breakfast, Lobby outside of seminar room	
9:05 – 9:35	Roaming Under the Microscope: Trajectory Study of Formaldehyde Dissociation	Paul Houston
9:35 – 10:05	Roaming Mechanisms for Nitrogen Containing Compounds: $\text{CH}_3\text{NO}_2$ , $(\text{CH}_3)_2\text{NNH}_2$ , $\text{CH}_3\text{NH}(\text{NO}_2)$ , and $\text{HNNOH}$	Stephen Klippenstein
10:10 – 10:35	Break (Refreshments), Lobby	
10:45 – 11:15	Patterns, Broken Patterns, and Broken Patterns of Broken Patterns	Bob Field
11:15 – 11:45	Rotationally Resolving Large Buffer-Gas Cooled Molecules In The Mid-infrared With Direct Frequency Comb Spectroscopy	Ben Spaun
11:45-noon	Additional discussion	
Noon – 1:30	Lunch in Emory Village	

PM Session Chairs: Joel Bowman and Balakrishnan Naduvalath

1:30 – 2:00	Towards Quantum-State-Resolved Charged-Neutral Chemistry	Eric Hudson
2:00 – 2:30	Competing Pathways in the Near-UV Photodissociation of Acetaldehyde	Craig Murray
2:30 – 3:00	Geometric Phase Effects Associated with Conical Intersections in the Ultracold Regime	Svetlana Kotochigova
3:00 – 3:30	Break (Refreshments)	
3:30 – 4:00	Roaming Signature in Photodissociation of Some Carbonyl Compounds	King-Chuen Lin
4:00 – 4:30	Quantum Dynamics of Cold Inelastic Diatom-Diatom Collisions in Full Dimensionality	Phillip Stancil
4:30 – 5:00	Roaming: Dynamical Reaction Pathways in Phase Space	Stephen Wiggins
6:30	Cocktails (cash bar) for all in the Starvine Ballroom at the Emory Conference Center Hotel (ECCH)	
7:00	Dinner for all registered, in the ECCH Starvine Ballroom	

ARO Workshop on Roaming and Cold Molecules Emory University, 360 Atwood Hall  Schedule for <b>SUNDAY</b> , Oct. 9, 2016		
AM Session Chairs: Gary Douberly and Francesco Evangelista		
8:00 – 8:30	Continental Breakfast	
8:30 – 9:00	Direct Dynamics Simulations of the Role of Microsolvation in $S_N2$ Reactions. Consideration of the Theoretical Method, Zero Point Energy, and Experiment	Bill Hase
9:00 – 9:30	Two-electron Reduced Density Matrices in Electronic Structure and Dynamics	David Mazziotti
9:30 – 10:00	Molecular Alignment Effect on the Photoassociation Process via a Pump-Dump Scheme	Yonchang Han
10:00 – 10:30	Break (Refreshments)	
10:30 – 11:00	Control of Roaming in Complex Organic Reactions in Solution	Dan Singleton
11:00 – 11:30	Including Roaming Trajectories Within the TST fold.	Rigoberto Hernandez
11:30-noon	Additional discussion	
Noon – 1:30	Lunch in Emory Village	
PM Session Chair: Michael Heaven		
1:30 – 2:00	Roaming in Coulomb Crystals	Ken Brown
2:00 – 2:30	Roaming in Biomolecular Reactions	Arthur Suits
2:30 – 3:00	Wrap up	

Onsite contact: Susan Browne, 404-377-6117 (cell), [sebrown@emory.edu](mailto:sebrown@emory.edu)



Attendees  
ARO Workshop on Roaming and Cold Molecules  
Emory University, Oct. 8-9, 2016

Name	Location
Chandika Amarasinghe	U. of Missouri
Timothy Barnum	MIT
Melissa Baudhuin	University of Minnesota
Louis Baum	Harvard University
Michael Berman	AFOSR
Joel Bowman	Emory University
Sean Bresler	Emory
Ken Brown	Ga Tech
Susan Browne	Emory University
Gary Chen	UCLA
Robin Côté	University of Connecticut
James Croft	University of Nevada, Las Vegas
Gary Douberly	University of Georgia
Tomoyuki Endo	INRS, Montreal
Francesco Evangelista	Emory University
Bob Field	MIT
Casey Foley	U. of Missouri
John Gray	JILA, University of Colorado
Ziwei Guo	Emory University
Yongchang Han	Dalian University of Technology
Bill Hase	Texas Tech
Michael Heaven	Emory University
Rigoberto Hernandez	Johns Hopkins
Paul Houston	Cornell University
Eric Hudson	UCLA
Abid Hussain	Univ Hamburg Germany
Jun Jiang	MIT
Steve Klippenstein	Argonne
Svetlana Kotochigova	Temple
Ivan Kozyryev	Harvard University
Ming Li	Temple University

Attendees  
ARO Workshop on Roaming and Cold Molecules  
Emory University, Oct. 8-9, 2016

King-Chuen Lin	Nat Taiwan U.
Xinyou Ma	Texas Tech University
Constantinos Makrides	Temple University
David Mazziotti	U. of Chicago
Michael Mills	UCLA
Craig Murray	University of California, Irvine
Balakrishnan Naduvalath	University of Nevada, Las Vegas
Apurba Nandi	Emory
Jim Parker	U.S. Army Research Office
Prateek Puri	UCLA
Chen Qu	Emory University
Philipp Schmid	JILA - University of Colorado
Dan Singelton	Texas A&M
Ben Spaun	JILA, University of Colorado
Phillip Stancil	University of Georgia
Arthur Suits	U. of Missouri
Michael N. Sullivan	Emory University
Azmain Taz	Emory University
Gideon Femi Tolufashe	University of KwaZulu
Brian Van Hoozen	Cornell University
Qingfeng (Kee) Wang	Emory University
Jonathan Weinstein	University of Nevada
Stephen Wiggins	Bristol
Tiangang Yang	UCLA
Benhui Yang	University of Georgia
Huan Yang	Shandong University
Qi Yu	Emory University

Updated 10/7/2016